X-MASS: A TOOL FOR SIMULTANEOUS CALCULATIONS OF CROSS-SECTIONS COVERING A LARGE PARAMETER SPACE FOR ATMOSPHERIC APPLICATIONS

VLADIMIR YU MAKHNEV, IOULI E GORDON, ROBERT J. HARGREAVES, LAURENCE S. ROTHMAN, *Atomic and Molecular Physics, Harvard-Smithsonian Center for Astrophysics, Cambridge, MA, USA*.

Reliable spectroscopic information, including that provided in the HITRAN database[a], is essential when interpreting data from high-resolution remote sensing spectrometers that monitor the concentrations of gases in the terrestrial atmosphere. High spectral resolution molecular absorption calculations over a wide spectral range and diverse parameter space using line-by-line models are often considered too slow to be used in operational retrieval algorithms. This is further slowed when using advanced line-shapes and line-mixing parametrizations that are available in HITRAN for many molecules (e.g. Hashemi et al.[b]), which are necessary for accuracy. As an alternative, retrieval codes often rely on massive sets of pre-calculated tables of absorption cross-sections for target molecules that cover a representative set of environmental conditions. For some missions, such as the NASA Orbiting Carbon Observatory (OCO-2/3)[c], molecular absorption coefficients are calculated off-line for a range of pressures, temperatures, and H_2O volume mixing ratios and stored in "ABSCO" lookup tables[d]. We present a Python tool (X-MASS) that allows the massive set of ABSCO tables to be calculated using the HAPI software package[e] with complete utilization of the parameters' accuracy in HITRAN, including sophisticated line shapes. The outputs will be made available in the convenient HDF5 or NetCDF formats given user-defined wavenumber step, set of pressures, temperatures, and diluent gas contents. X-MASS will be an open-source library where users can specify parameters for their applications. In addition, a set of pre-calculated ABSCO tables covering spectral range of molecules at a finer grid and resolution will be provided on the HITRAN website. This work will facilitate the timely integration of state-of-the-art spectroscopic data into atmospheric radiative transfer codes.

---

[a] Gordon, I. E., *et al.* JQSRT 277 (2022): 107949.

[b] Hashemi, R., *et al.* JQSRT 271 (2021): 107735.

[c] Crisp, D., *et al.* Atmospheric Measurement Techniques 10.1 (2017): 59-81.

[d] Payne, V.H., *et al.* JQSRT 255 (2020): 107217.

[e] Kochanov, R.V., *et al.* JQSRT 177 (2016): 15-30.